Effects of LES sub-grid flow structure on particle deposition
in a plane channel with a ribbed wall

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SUMMARY

Transport and deposition of aerosol particles in a plane channel with a ribbed wall are studied in order to investigate the effects of the turbulent flow structure on particle deposition. In this paper, kinematic simulation (KS) has been adapted to be a sub-grid model for particles, in conjunction with large eddy simulation (LES) in real space with boundaries. KS is a Lagrangian model of turbulent dispersion that takes into account the effects of spatio-temporal flow structure on particle dispersion. It is a unified Lagrangian model of one-, two- and indeed multi-particle turbulent dispersion and can easily be used as a Lagrangian sub-grid model for LES codes, thus enabling complex geometry to be taken into account. To study the effect of small-scale flow structures on particle deposition in the ribbed channel flow, we use a validated LES code to simulate the flow field, and KS to model the sub-grid flow structures. Thus, the large scales are resolved by the simulation and the small scales are modelled using various sub-grid models. As none of the existing sub-grid models is known to have taken into account the effects of small-scale turbulent flow structures on particle deposition, it is important to use KS’s ability to remodel the sub-grid velocity field and thereby incorporate its effect on particle deposition. The parameters of our simulations for LES are the Reynolds number, width of the channel, height of the rib and sub-grid model parameters. For KS, the parameters are the energy dissipation rate obtained from LES, the energy spectra, ratio of the largest and smallest sub-grid scales and the total number of modes for the sub-grid velocity field. The turbulent flow features thus obtained are compared with published experimental data in a ribbed channel. Our results suggest that while the small-scale (sub-grid) turbulent flow structures have negligible effects on particles with large relaxation times (compared with the Kolmogorov dissipation time scale), deposition of the particles with small relaxation times in the ribbed channel can be affected by these sub-grids. Copyright © 2008 John Wiley & Sons, Ltd.

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1. INTRODUCTION

Particle-laden flows are ubiquitous in nature. They appear in many fields of engineering, ranging from the pollutant dispersion in air or water for environmental applications, to transport of contaminants in industrial processes and also in the human airway [1]. Understanding and quantitative assessment of local air flow fields and micron-particle deposition distributions in tracheo-bronchial airway are highly important for estimating the effect of certain inhaled pollutants and the efficiency of the delivery of aerosol drugs, such as those used to treat airway inflammation in asthma patients. Balashazy et al. [2] pointed out that local-particle deposition patterns may play a key role in the development of lung cancer. To determine the local-particle depositions by in vivo or in vitro tests is very difficult and cost intensive. Hence, validated computational fluid dynamics (CFD) simulations can provide us with a non-invasive, accurate and cost-effective means to obtain such information. A number of works have been done on the problem of air flow and particle deposition in airway models using CFD techniques [3–7].

A reliable estimation of particle deposition in the human airway requires an understanding of the underlying flow structures and the effect of these structures on particle dispersion. Most of the works on airway–particle transport assumes a simplified approximation of the flow field [1, 8], but experimental measurements indicate Reynolds numbers (Re) approaching as high as 9300 [9]. This indicates that modelling the effect of turbulence on particle deposition is relevant and important.

Turbulent flows are characterized by the presence of a broad range of spatial and temporal scales of motion. These scales of motion are typically known as eddies. The largest of these eddies are directly related to the size of the flow domain, whereas the smallest length scales (the Kolmogorov scale) are responsible for the dissipation of the kinetic energy into heat through viscosity.

To study the turbulent transport of particles in a complicated structure, such as the human airway, is extremely difficult [3], as is modelling turbulent flows. It is likewise rather daunting to include the effects of turbulence on particle trajectories in a complicated geometry. Most of the CFD work in the field of airway–particle deposition assumes either a simple geometry [10] or laminar flow with complicated geometry [5], although in the context of industrial or engineering studies, there are investigations on turbulent particle deposition involving complicated geometry [11]. Despite its importance, to date, only limited work has been done to understand the effects of turbulent flow modelling on particle deposition. Kleinstreuer and Zhang [12] used a low Reynolds number k–ω model to capture the effect of turbulent flow on particle deposition in the airway. Lo Iacono et al. [13, 14] predicted particle deposition from large eddy simulation (LES) of ribbed channel flow. In these models, the sub-grid model is either modelled stochastically or ignored, as their effects on particles with relatively greater relaxation time are considered negligible. Recently, more advanced LES modelling has been developed for tracking particles in turbulent flows by Shotorban and Mashayek [15] and Kureten and Vreman [16], where an inverse filtering model is proposed and incorporated into the particle equations. They have shown that this can enhance the turbophoresis in actual LES and improve the agreement with direct numerical simulation (DNS). However, these models still cannot recover the effects of ‘unrepresented’ modes, which are lost in...
EFFECTS OF LES SUB-GRID FLOW STRUCTURE

LES. Armenio et al. [17] have shown that the effect of sub-grid velocity fields is important, and neglecting these effects on particle trajectories could introduce errors into particle statistics.

In order to provide a model that captures the salient features of the sub-grid velocity field and show their effect on particle statistics, in this paper, we use the kinematic simulation (KS) [18, 19] to model the sub-grid velocity field and investigate the effects on particle dispersion and deposition in a ribbed channel (see, Figure 1) turbulent flow.

The idea and technique behind KS have been around for some time now. Several papers have been published using this technique to elucidate the effects of turbulent flow structures on particle dispersion. LES has also been extensively studied in the last few years as an alternative for turbulent flows in a complex geometry. KS is simple, much cheaper to use, but is currently mostly applied in homogeneous turbulent flow. The new contribution here, to the best of our knowledge, is that this is the first time that KS has been adapted to be a sub-grid model for particles in conjunction with an LES simulation in real space with boundaries. The only previous work that used KS as a sub-grid model was in the context of spectral space LES simulation for homogeneous and isotropic velocity field without boundaries [20]. If this is successful, then the idea can be extended to other more complex turbulent flows, such as airway flows.

It is worth pointing out that the use of the KS model has in many instances reproduced DNS and experimental results successfully [21–23]. KS was constructed as a Lagrangian model of turbulent dispersion of particles. In this context, apart from using DNS itself, which is often beyond one’s computational power for many realistic problems, employing KS with LES is in principle more advanced compared with tracking particles using Reynolds-averaged Navier–Stokes (RANS) or LES only (in which case the small eddy effects are simply ignored, e.g. [24]), or RANS/LES plus stochastic models (in which case the SGS is disconnected from the particle’s model, e.g. [25]).

It is also noted that it is not our intention to develop a better LES model in this paper; rather the focus is on adapting the KS model within an LES model, assuming that turbulence flow modelling is taken care of by a valid LES. In other words, we do not address the modelling errors in LES, since our KS model can in principle be implemented in any LES model, including the LES model with inverse filtering [16], since in these types of models, the ‘unrepresented modes’ are still uncovered. For the ribbed channel flow presented in this paper, the LES model has been used extensively tested against experiments [13], and all small eddies above cut-off are captured by LES. Thus, only the...
even smaller eddies, which are considered to be homogeneous, are modelled by KS. The energy spectrum in the sub-grid is controlled by the smallest grid size and the turbulent dissipation scale, and it is present only far away from the walls. The amount of sub-grid contribution is controlled by the magnitude of sub-grid dissipation $\varepsilon$, which varies with the distance from the wall and also by the viscous cut-off length $\eta$.

2. LARGE EDDY SIMULATION (LES)

The idea behind LES is to compute exactly the mean flow field and the large energy-containing scales of motion; the small-scale flow structures/scales of motion are not simulated, but their influence on the rest of the flow is parameterized by some heuristic models. In other words, LES decomposes the flow field into resolved/grid scales (GS) associated with the large or energy-containing scales, and small sub-grid scales (SGS) related to the universal smaller scales, which are modelled [26]. The resolved scales of motion $\mathbf{F}$ are obtained through filtering the flow variables in the following way:

$$\mathbf{F}(\mathbf{x}) = \mathbf{G} * \mathbf{F} = \int_{\Omega} \mathbf{F}(\mathbf{x}') \mathbf{G}(\mathbf{x}, \mathbf{x}', \Delta) \, d\mathbf{x}'$$

where $\mathbf{F}$ represents the flow variables (velocity $\mathbf{u}$, pressure $p$, etc.), $*$ denotes the convolution product, $\Omega$ is the computational domain, $\mathbf{G}$ is the filter function and it is a function of $\mathbf{x}$ and $\mathbf{x}'$ the position vectors and $\Delta$; the filter width here is chosen to be equal to the grid resolution or size. The filter function or the kernel $\mathbf{G}$ has the following properties [27, 28]:

$$\int_{\Omega} \mathbf{G}(\mathbf{x}, \mathbf{x}', \Delta) \, d\mathbf{x}' = 1, \quad \mathbf{G} = \mathbf{G}(|\mathbf{x} - \mathbf{x}'|, \Delta)$$

$$\lim_{\Delta \to 0} \mathbf{G}(\mathbf{x}, \mathbf{x}', \Delta) = \delta(\mathbf{x} - \mathbf{x}') \quad \text{and} \quad \mathbf{G}(\mathbf{x}, \mathbf{x}', \Delta) \in C^0(\mathbb{R}^3)$$

with compact support. Any function having the above properties can be used as a filter function. The first constraint in (2) imposes normalization, whereas the second constraint is the requirement that the function is symmetric and only depends on the magnitude of $\mathbf{x} - \mathbf{x}'$. The third constraint is the requirement that the effect of the grid must vanish as $\Delta \to 0$, implying that the filtered Navier–Stokes equation (NSE) approaches the unfiltered NSE as the grid is refined. The fourth constraint extends the concept of a filter to include distributions [29].

Convolving the NSE and continuity equation with $\mathbf{G}$ and assuming that the filter function commutes with temporal $\partial_t$ and spatial $\nabla$ derivatives, i.e. $[\mathbf{G}, \partial_t] \mathbf{v} = 0$ and $[\mathbf{G}, \nabla] \mathbf{v} = 0$ (the commutation relation for the spatial derivatives is not true for non-uniform grids, which we have used in our simulation, but the errors thus introduced can be considered negligible in the light of our second-order discretization scheme [30]), we get the following filtered equations for the fluid [27]:

$$\frac{\partial \mathbf{u}_i}{\partial x_i} = 0$$

$$\frac{\partial \mathbf{u}_i}{\partial t} + \frac{\partial}{\partial x_j} (\mathbf{u}_i \mathbf{u}_j) = -\frac{1}{\rho_i} \frac{\partial p}{\partial x_i} + \frac{\mu}{\rho_i} \frac{\partial}{\partial x_j} \left( \frac{\partial \mathbf{u}_i}{\partial x_j} + \frac{\partial \mathbf{u}_j}{\partial x_i} \right) - \frac{\partial \tau_{ij}}{\partial x_j}$$
where \( \tau_{ij} = \overline{u_i u_j} - \overline{u_i} \overline{u_j} \) is the SGS stress, representing the interaction between small and resolved large scales of motion. In addition, \( \rho_T \) and \( \mu \) are the fluid’s density and viscosity, respectively. The basic problem of LES is to find an appropriate model for the SGS stresses represented by \( \tau_{ij} \), expressed in terms of the large-scale field or the GS fields. The sub-grid modelling basically includes the filtered equations of motion a way to transfer the kinetic energy from the large scales towards the SGS, where it is eventually dissipated by molecular viscosity. In the absence of any sub-grid transfer, there will be an accumulation of energy at the cut-off length scale, i.e. at the smallest grid size \( \Delta \), while the presence of a pile up depends on the type of numerical discretization that can add artificial viscosity. This kind of problem is referred to as a problem of homogenization in Mathematics [26].

A simple example of an SGS model is that of Smagorinsky [31], where the SGS stress is parameterized using the eddy viscosity hypothesis, as \( \tau_{ij} = 2 \nu_T \overline{\sigma_{ij}} \), where the eddy viscosity is \( \nu_T = C \Delta^3 | \overline{\sigma} | \), and \( \overline{\sigma_{ij}} = (\partial \overline{u_i}/\partial x_j + \partial \overline{u_j}/\partial x_i) \) is the resolved scale or GS velocity field strain rate tensor. Here, \( | \overline{\sigma} | = \sqrt{\overline{\sigma_{ij}} \overline{\sigma_{ij}}} \) is the magnitude of \( \overline{\sigma_{ij}} \). The filter width \( \Delta \) is defined as \( \Delta = (\Delta_x \Delta_y \Delta_z)^{1/3} \), where \( \Delta_x, \Delta_y, \Delta_z \) are the grid spacings in the \( x, y \) and \( z \) directions, respectively.

We use the zonal \( k-l \) based LES of Tucker et al. [32]. This LES code besides solving for the filtered velocity field also solves the transport equation for the turbulent kinetic energy \( k_T \) and uses RANS modelling near the wall. The interface location for these two models is either explicitly specified based on the physics of turbulence or grid controlled. The simple Yoshizawa \( k-l \) [33, 34] model for SGS modelling is used in the LES region away from the wall for the Eulerian velocity field. The modelled turbulent kinetic energy is governed by the following transport equation:

\[
\frac{\partial k_T}{\partial t} + \frac{\partial \overline{u_i k_T}}{\partial x_i} = \frac{1}{\rho} \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_T}{\sigma_k} \right) \frac{\partial k_T}{\partial x_j} \right] + P_{kT} - \varepsilon_{T}
\]  

(5)

where \( \sigma_k = 1 \) is the diffusion Prandtl number for \( k_T \), and \( P_{kT} \) is the turbulence production term. The subscript \( i \) is used to differentiate between LES- and RANS-related components. In the RANS region, \( \mu_T = \mu \) the eddy viscosity, and for the LES region \( \mu_T = \muSGS \), the SGS viscosity. In this model, the eddy viscosity and dissipation rate are given by \( \mu_T = \rho C_{\mu1} l_\mu k_T^{1/2} \) and \( \varepsilon_T = C_{\varepsilon1} k_T^{3/2}/l_\varepsilon \), respectively, where \( C_{\mu1} \) and \( C_{\varepsilon1} \) are turbulence modelling constants [32]. \( l_\mu \) and \( l_\varepsilon \) are length scales related to the filter width \( \Delta \) via the following relations [32]:

\[
l_\mu = n C_{\mu2} y (1 - e^{-A_\mu y^*}) + (1 - n) \Delta
\]  

(6)

\[
l_\varepsilon = n C_{\varepsilon2} y (1 - e^{-A_\varepsilon y^*}) + (1 - n) \Delta
\]  

(7)

where \( y^* = y \rho k_T^{1/2}/\mu \), \( n = 0 \) or 1 activates LES or RANS modelling, and the \( n \) switch location is based on turbulence flow physics. To control the switching via the grid, the following relations are used instead:

\[
l_\mu = \text{min}\{C_{\mu2} y (1 - e^{-A_\mu y^*}), \Delta\}
\]  

(8)

\[
l_\varepsilon = \text{min}\{C_{\varepsilon2} y (1 - e^{-A_\varepsilon y^*}), \Delta\}
\]  

(9)
Table I. Turbulence modelling constants [32].

<table>
<thead>
<tr>
<th>Model</th>
<th>n</th>
<th>A_n</th>
<th>A_μ</th>
<th>C_1</th>
<th>C_2</th>
<th>C_μ1</th>
<th>C_μ2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wolfshtein et al.</td>
<td>1</td>
<td>0.263</td>
<td>0.0160</td>
<td>1</td>
<td>2.400</td>
<td>0.09</td>
<td>2.400</td>
</tr>
<tr>
<td>Chen et al.</td>
<td>1</td>
<td>0.200</td>
<td>0.0143</td>
<td>1</td>
<td>2.495</td>
<td>0.09</td>
<td>2.495</td>
</tr>
<tr>
<td>Yoshizawa/Fureby</td>
<td>0</td>
<td>—</td>
<td>—</td>
<td>1.05</td>
<td>—</td>
<td>0.07</td>
<td>—</td>
</tr>
</tbody>
</table>

Table II. Computational domain and simulation parameters.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reference velocity ( u_0 )</td>
<td>3.6 (m/s)</td>
</tr>
<tr>
<td>Friction velocity ( u_\tau )</td>
<td>0.595 (m/s)</td>
</tr>
<tr>
<td>Fluid density ( \rho_f )</td>
<td>1.2 (kg/m(^3))</td>
</tr>
<tr>
<td>Fluid Viscosity ( \mu )</td>
<td>( 1.83 \times 10^{-5} ) (kg/m(s))</td>
</tr>
<tr>
<td>Height of the rib ( h )</td>
<td>0.00635 m</td>
</tr>
<tr>
<td>Channel half width ( \delta = L_y / 2 )</td>
<td>5( h )</td>
</tr>
<tr>
<td>Stream-wise dimension ( L_x )</td>
<td>( 20h = 67% ) ( 2\pi ) ( \delta )</td>
</tr>
<tr>
<td>Span-wise dimension ( L_z )</td>
<td>( 10h = 64% ) ( \pi ) ( \delta )</td>
</tr>
<tr>
<td>Reynolds number ( Re = u_0 \delta / \nu )</td>
<td>7000</td>
</tr>
<tr>
<td>Number of grid points</td>
<td>121 \times 112 \times 33</td>
</tr>
<tr>
<td>Number of grid points (finer mesh)</td>
<td>121 \times 112 \times 67</td>
</tr>
<tr>
<td>Kolmogorov dissipation time ( t_\eta = T / Re^{1/2} )</td>
<td>4.23 \times 10^{-4} s</td>
</tr>
<tr>
<td>( T = L_x / u_0 )</td>
<td></td>
</tr>
<tr>
<td>Time step ( \Delta t )</td>
<td>1.0 \times 10^{-4} s</td>
</tr>
<tr>
<td>Particle density ( \rho_p )</td>
<td>500, 10000 kg/m(^3)</td>
</tr>
<tr>
<td>Particle diameter ( d_p )</td>
<td>87.0, 8.7 ( \mu ) ( m ) ( \times 10^{-6} ) m</td>
</tr>
<tr>
<td>Particle relaxation time ( \tau_p )</td>
<td>0.0115, 0.023, 0.00023 s</td>
</tr>
<tr>
<td>( \tau_p / t_\eta )</td>
<td>0.54, 27.27, 54.54</td>
</tr>
<tr>
<td>Number of particles tracked</td>
<td>10000</td>
</tr>
</tbody>
</table>

In this paper we use the turbulence flow physics based switching between LES and RANS near the wall, and the \( n \) switch location is explicitly set to 10% of the rib height \( h \) [32]. This means that near the wall at distances less than 0.1\( h \) LES is switched off and RANS is activated. Tucker and Davidson [32] have shown that this choice of switching between LES and RANS gives results that are in better agreement with experimental measurements (Table I).

The governing equations are discretized in a centred, second-order, staggered grid finite difference frame work. The Crank–Nicholson scheme was used to integrate the flow equations in time. Integration time steps are taken to be much smaller than the Kolmogorov dissipation timescale \( t_\eta = T / Re^{1/2} \), where \( T \) is the turnover (or evolution) time of the largest eddies of size \( L_x \) [13]. At solid walls, a no-slip boundary condition is applied. Periodic boundary conditions are applied at non-solid walls. A geometrical expansion is used for our non-uniform grids containing 121 \times 112 \times 33 (and 67) (see Table II) elements. The spacing between the consecutive grid points (i.e. mesh size) in the \( x \), \( y \) and \( z \) directions are \( 13\leq \Delta^+ \leq 76 \), \( 6\leq \Delta^+ \leq 60 \), \( \Delta^+ \sim 70 \) (and 35), expressed here in terms of dimensionless wall units [35]. Where the \( + \) sign indicates that the quantities have been non-dimensionalized using the wall friction velocity \( u_\tau \) and the fluid viscosity \( \mu \) [35].
3. PARTICLE PHASE MODELLING

The common practice when using LES to study particle-laden turbulent flows is to solve the Lagrangian equations of motion and track the individual particles. The particles are usually assumed to be smaller than the smallest scales of the turbulent flow, i.e. the Kolmogorov scale. The forces that act on them are the forces due to the pressure gradient of the fluid, the viscous drag, viscous stresses, the inertia force of the added mass, the Basset force and the buoyancy force [36]. All these forces except the buoyancy force are functions of the instantaneous velocity field of the fluid. But in a LES simulation these are absent, so one resorts to using the filtered velocity field to calculate these forces, thus neglecting the effect of the sub-grid or filtered out velocity field on the particle trajectories [15,17]. The authors in [15,17] have been able to show that this results in computed particle trajectories and statistics having errors, which increase as the filter gets coarser or the particle relaxation time gets smaller. For a spherical particle, the relaxation time is defined as 

\[
\tau_p = \frac{4 \rho_p d_p^2}{3 \mu C_d Re_p} \]

[37], where \( \rho_p \) and \( d_p \) are the density and diameter of the particle and \( \mu \) is the viscosity of the fluid. \( C_d \) is the drag coefficient, given by 

\[
C_d = \frac{24}{Re_p} \text{ if } 0 < Re_p < 0.5, \quad C_d = (24/Re_p)(1 + 0.15Re_p^{0.687}) \text{ if } 0.5 < Re_p < 10^3 \]  

[37]. In the former expressions, \( Re_p \) is the particle Reynolds number defined as \( Re_p = \rho_l |(u_p - u_f)| d_p / \mu \), where \( u_p \) and \( u_f \) are the particle and the local fluid velocity, respectively, and \( \rho_l \) is the fluid density. In this paper, we consider heavy spherical particles advected by the instantaneous velocity field of a turbulent flow, which consists of the filtered velocity field \( \mathbf{u}_{LES} = \mathbf{u} \) simulated by LES and of a sub-grid velocity field \( \mathbf{u}_{KS} \) modelled by KS (see, Section 4). The particles are assumed to have no effect on the flow field. The particle equation of motion is assumed to be given by (10), where the dominant governing forces are the drag \( \mathbf{F}_{\text{Drag}} \), gravity and Saffman lift.

\[
m_p \frac{d \mathbf{u}_p}{dt} = \frac{1}{2} \rho_l C_d A |\mathbf{u}_p - \mathbf{u}_f| (\mathbf{u}_p - \mathbf{u}_f) + m_p \mathbf{g} + \mathbf{L}_{\text{Saff}}
\]

(10)

where \( \mathbf{g} \) is the acceleration due to gravity, \( A = \pi d_p^2 / 4 \) is the projected area of the particles and the Saffman lift term \( \mathbf{L}_{\text{Saff}} \) [38] is given by

\[
\mathbf{L}_{\text{Saff}} = 1.615 \ d_p^2 (\rho_l \mu)^{1/2} \left( \frac{1}{|\mathbf{\omega}_f|} \right)^{1/2} (\mathbf{u}_p - \mathbf{u}_f) \times \mathbf{\omega}_f \mathcal{F}
\]

(11)

where \( \mathbf{\omega}_f = \nabla \times \mathbf{u}_f \) is the fluid vorticity, \( \mathcal{F} \) is the high \( Re_p \) correction function of Mei [38]. The latter extends the validity of Equation (11) to the range \( 0 < Re_p < 100 \). Less dominant terms such as the Faxen correction to Stokes drag, the added mass, Basset history and buoyancy are neglected in favour of the dominant drag force. This is because of the assumed large particle density \( \rho_p \) compared with the fluid density (i.e. \( \rho_p / \rho_l \gg 1 \)) and the relatively small particle diameter [36]. As highlighted by McLaughlin [10], the Saffmann lift, although small compared with the drag, is significant in the viscous sub-layer near the wall. This is due to the high shear affecting the particle deposition, and therefore we include the lift in our governing equation. More detailed information can be found in [36,39,40].

In total 10000 particles were released into the mature LES flow from random locations on the wall-parallel plane \((x,z)\) in the centre of the channel (i.e. \( y/h = 4.8 \)) with velocity equal to the
local fluid’s velocity. This corresponds to an initial volume particle fraction of order $O(10^{-6})$ and makes appropriate to adopt one-way coupling, i.e. fluid–particle and particle–particle interactions are ignored. A particle is assumed to be deposited and remains so at subsequent times, when its centre of mass is located at a distance from the wall, less than or equal to the particle’s radius. If a particle leaves the computational domain at one side, (in the $x$ or $z$ direction) it is reintroduced at the corresponding point on the opposite face of the flow domain. Particles that deposit are not replaced. The particle equations of motion (10) are integrated using a fourth-order Runge–Kutta method. A sixth-order Lagrangian interpolation is used to evaluate the instantaneous velocity of the fluid at the particle locations [13].

4. KS AS A SUB-GRID MODEL OF THE VELOCITY FIELD IN LES

KS is a Lagrangian model of turbulent dispersion that takes into account the effects of spatio-temporal flow structure on particle dispersion [41]. The idea was based on Kraichnan’s model for single-particle diffusion in an incompressible, isotropic velocity field (albeit non-turbulent) using a finite number of random Fourier modes [42]. It is a direct Lagrangian, purpose built, model that is very robust and can be used in fully turbulent flow or transitional flows. It is a unified Lagrangian model of one-, two- and indeed multi-particle [22] turbulent dispersion. It can be easily used as a sub-grid model [20] for LES code thus enabling complex geometry to be taken into account.

We describe the construction of such model velocity field in the light of [20, 21, 41], which has the properties usually associated with turbulence. It differs completely from dynamical simulation, such as DNS, RANS and LES, which solves numerically either the full, averaged or filtered NSE on a grid of points all over the domain of calculation. However, in KS, the dynamics of the flow is not modelled. Instead, the time evolution of the velocity field is prescribed through a set of frequencies $\omega_n$, which will be discussed later. Since there is no energy transfer or dissipation in KS, we can formally define the energy dissipation rate based on the prescribed energy spectrum $E(k)$ in our simulation. The character of the flow is then determined by the energy spectrum. Hence, the type of flow can be changed easily by changing the spectrum. The advantage of KS is that it elucidates the Lagrangian properties of particle dispersion with a given Eulerian flow field and connects these properties with the Eulerian structures present in the velocity field. Being non-Markovian, it also introduces some persistence of these structures [41].

The KS method is far cheaper computationally than traditional DNS, which requires a huge number of modes and cannot simulate high Reynolds number flows. At the same time, KS has the ability to reproduce DNS results with fewer modes (four orders of magnitude less [21]) and also simulate extremely high Reynolds number flows.

Given the turbulent energy spectrum of the flow $E(k)$, the velocity field in two or three dimension $\mathbf{u}_{KS}(\mathbf{x}, t)$ is simulated in KS by a large number of random orthogonal Fourier modes varying in space and time over a large number of realizations. The prescribed Eulerian properties of the generated velocity field are

1. Incompressibility $\nabla \cdot \mathbf{u}_{KS}(\mathbf{x}, t) = 0$.
2. Energy spectrum $E(k) \sim k^{-p}$; $1 < p < 2$.
3. Existence of eddying and streaming flow structures and
4. Time-dependence of these structures determined by $\omega_n$. 

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Individual realizations of an Eulerian turbulent-like velocity field $\mathbf{u}_{KS}(x, t)$ are generated as follows:

$$\mathbf{u}_{KS}(x, t) = \sum_{n=1}^{N_k} [A_n \wedge \mathbf{k}_n \cos(\mathbf{k}_n \cdot \mathbf{x} + \omega_n t) + B_n \wedge \mathbf{k}_n \sin(\mathbf{k}_n \cdot \mathbf{x} + \omega_n t)]$$

where $\wedge$ means vector cross product between the vectors, $N_k$ is the number of modes in the simulations and $\mathbf{k}_n$ is the wave vectors. The incompressibility condition implies

$$A_n \cdot \mathbf{k}_n = B_n \cdot \mathbf{k}_n = 0$$

The positive amplitudes $|A_n| = A_n$ and $|B_n| = B_n$ are chosen according to

$$A_n^2 = B_n^2 = 2E(k_n)\Delta k_n$$

where $k_n = |\mathbf{k}_n|$, $E(k)$ is a prescribed Eulerian energy spectrum of the form:

$$E(k) = E_0 L(k L)^{-\beta}$$

in the range $k_L = 2\pi/L = k_1 \leq k \leq k_N = 2\pi/\eta = k_0$, such that $E(k) = 0$ outside this range. Here, $E_0$ is a constant with the dimensions of energy, $L$ and $\eta$ are the largest and the smallest spatial scales of the velocity field where it obeys the above spectrum. $\Delta k_n = (k_{n+1} - k_n)/2$ for $2 \leq N_k \leq N_k - 1$, $\Delta k_1 = (k_2 - k_1)/2$ and $\Delta k_{N_k} = (k_{N_k} - k_{N_k - 1})/2$. The distribution of the wave numbers $k_n$ is either linear, algebraic or geometric, i.e.

$$k_n = \begin{cases} k_1 + \left(\frac{k_n - k_1}{N_k - 1}\right)(n - 1) & \text{(Linear)} \\ k_1 n^x & \text{(Algebraic)} \\ k_1 a^{n-1} & \text{(Geometric)} \end{cases}$$

where $x$ and $a$ are dimensionless numbers that are functions of $L/\eta$ and $N_k$, because $k_{N_k} = 2\pi/\eta$. Hence, $x = \ln(L/\eta) / \ln N_k$, and $a = (L/\eta)^{1/(N_k - 1)}$, respectively. We have used the geometric distribution of modes, which leads to equally spaced modes over different energy shells in log scale. The linear distribution has most of the modes packed in the large wave number regime, whereas the geometric distribution is somewhere in between. The reason behind using this distribution of modes is due to the fast convergence and insignificant variation of statistics with the number of modes $N_k$ (small $O(10)$) or large $O(100)$) used [20] in the simulation. This allowed us to use fewer modes ($\sim 40$) that made the calculations computationally inexpensive. The frequencies $\omega_n$ determine the unsteadiness associated with the wave mode $n$. In our present simulation, we have used $\omega_n$ to be proportional to the eddy turnover frequency of the $n$th wave mode $k_n$, i.e.

$$\omega_n = \lambda \sqrt{k_n^3 E(k_n)}$$

The dimensionless unsteadiness parameter $\lambda$ by which all frequencies $\omega_n$ are multiplied as in Equation (16) serves to investigate the effect of unsteadiness of the velocity field. Large values of $\lambda$ correspond to short correlation times compared with the eddy turn over time $2\pi/\sqrt{k_n^3 E(k_n)}$. The effect of large $\lambda$ could also be likened to a Doppler shift of the frequencies $\omega_n$. In this case, the local velocity behaviour becomes chaotic/random while $\lambda = 0$ corresponds to a frozen velocity field. In a steady ($\lambda = 0$), two-dimensional flow, particle trajectories follow closed streamlines most
of the time and the flow field do not evolve in time but remain frozen (due to the absence of dynamics in KS). However in three dimensions, due to the presence of the third component of the velocity field, streamlines become chaotic and non-closed arising from the advective action of the third component on the rest. Hence, in two dimensions $\lambda=0$ is a special case with no dynamical evolution or turbulence, whereas in three dimensions it is possible to have dynamics even with $\lambda=0$; Hence, we use this value throughout our computations. In our computations, we use the prescribed Eulerian energy spectrum of the form:

$$E(k) = C_K \varepsilon_{KS}^{2/3} k^{-5/3}$$

where $C_K = 1.5$ is the Kolmogorov dimensionless constant \([43, 44]\), $\varepsilon_{KS}$ is a constant with dimensions of dissipation rate and $k_L, k_\eta$ define the range of wave numbers, where the random velocity field obeys the $-\frac{5}{3}$ inertial range scaling law.

Research \([19–21, 45]\) suggests that from a rather crude assumption of the form of the Eulerian velocity field, KS reproduces many relevant geometrical features of Lagrangian turbulence that have significant qualitative and quantitative implications on particle concentration and deposition. Comparisons of DNS results for two-particle statistics in stationary isotropic turbulence have shown good agreement with KS \([21]\). It was found that KS models reproduce well the global statistical properties of Lagrangian intermittency at the Reynolds numbers attainable by DNS. In KS, as in DNS and real turbulent flows, the non-Markovian geometry of trajectories is determined by the eddying, straining and perhaps also other structures in individual Eulerian realizations.

5. COUPLING LES AND KS

In the case of spectral space simulation of homogeneous isotropic turbulence, Flohr and Vassilicos \([20]\) coupled the LES and KS purely at the energy level (see Figure 2) by matching the rate of dissipation $\varepsilon_{LES}$ of the LES field with the dissipation-like parameter $\varepsilon_{KS}$ in the KS field. The
dissipation rate in the LES field is estimated using

\[ \varepsilon_{\text{LES}} = -\frac{dE(t)}{dt} \]  

(18)

where \( E(t) \) is the total kinetic energy of the resolved scales at time \( t \). This \( \varepsilon_{\text{LES}} \) is set equal to the parameter \( \varepsilon_{\text{KS}} \) in the sub-grid energy spectrum equation (4) of the kinematic field, where \( k_L \) in Equation (4) is now set equal to the LES cut-off wave number \( k_c \sim 1/\Delta \) (\( \Delta = (\Delta x \Delta y \Delta z)^{1/3} \) is the smallest grid spacing) and \( \varepsilon_{\text{KS}} = \varepsilon_{\text{LES}} \). The wave numbers \( k < k_c \) are correlated via the LES evolution equation, namely the NSE; however, none of the wave numbers \( k > k_c \) is correlated with each other, but are chosen independently from each other in the kinematic field. Therefore, we do not have any correlation between the kinematic modes and the LES field, which means that our sub-grid modelling is explicitly constructed for Lagrangian particle dynamics, but not for modelling the SGS of the Eulerian velocity field of LES. This is the main difference between the traditional approach of sub-grid modelling of the Eulerian velocity field and our approach.

Note that in general, for an inhomogeneous flow, the \(-5/3\) energy scaling may not necessarily be reproduced by the spectra of the filtered LES (although, we repeat, our LES model has be carefully validated). The \(-5/3\) energy scaling can indeed be reproduced by the spectra of the filtered LES for homogeneous flow [14]. However, our KS model is applied individually for all cells, and therefore the cut-off level is different for different cells. And on the individual grid level (below cut-off), this discontinuity is assumed to be small, which, after all, is the basic assumption of LES modelling. Even with this possible discontinuity, including this cut-off energy is still better than many current approaches, such as LES/RANS alone, or LES/RANS with a stochastic model, where this energy is simply ignored or independently approximated. In these the discontinuity would be greater.

The particle trajectories are calculated by integrating the following equations:

\[
\frac{dx_p}{dt} = u_p \\
\frac{du_p}{dt} = \frac{(u_p - u_f)}{\tau_p} + F_b
\]  

(19)  

(20)

where Equation (20) is just Equation (10) written in a compact form with \( F_b \) denoting all the body forces appearing in Equation (10). Here, the fluid velocity is given by \( u_f = u_{\text{LES}} + u_{\text{KS}} \), with \( u_{\text{LES}} \) obtained by solving Equation (3) and \( u_{\text{KS}} \) is given by Equation (12). In order to estimate the flux of energy to the SGS, we need to compute \( \varepsilon_{\text{LES}} \). The calculation depends on how the sub-grid modelling is done for the LES field. For example, if we compute the sub-grid viscosity \( \nu_{\text{SGS}} \) using the Smagorinsky’s model then we could use the following to estimate the energy flux from the resolved scales to the SGS:

\[ \varepsilon_{\text{LES}} = 2\nu_{\text{SGS}} \langle |\overline{S}|^2 \rangle, \quad |\overline{S}| = \sqrt{2 \overline{S}_{ij} \overline{S}_{ij}} \]  

(21)

where \( \langle \cdots \rangle \) implies ensemble averaging over many flow realizations and \( \langle \cdots \rangle \) means filtered quantities (see, Section 2). To estimate the sub-grid dissipation rate, we simply equate the above to \( \varepsilon_{\text{KS}} \). Different models exist in the literature relating \( \nu_{\text{SGS}} \) and \( \varepsilon_{\text{LES}} \); the simplest of them assumes a local equilibrium between the rate of injected energy \( \varepsilon_l \) at the large energy-containing scales, the transfer rate \( \varepsilon_T \) through the cut-off wave number \( k_c \) and the dissipation rate due to viscous
effects $\varepsilon$. This is expressed by the equality \[ I = T = \varepsilon \] (22)

Using the above relation and dimensional arguments \[ I \], one can derive the relationship between $v_{SGS}$ and $v_{LES}$ as shown in Equation (21). In our present work, we use the Yoshizawa $k-l$ model \[ k-l \] for the sub-grid modelling for the velocity field in the LES model. Therefore, we use the following simplified relation between the sub-grid energy flux and the resolved velocity field:

\[ \varepsilon_{KS} = \varepsilon_{LES} = \frac{k_e^{3/2}}{l_\mu} \] (23)

where $k_e$ is the kinetic energy of the resolved or GS velocity field, and $l_\mu$ is related to the filter width $\Delta$ \[ 32 \].

5.1. Sub-grid modelling for Lagrangian particle dispersion

We modify the LES velocity field seen by the particles, by adding the contribution from the SGS of motion via KS modelling. We have to adapt the global method of Flohr and Vessilicos \[ 20 \] to a non-uniform grid. In practice, we have to apply their method locally to each and every grid cell of the discretized flow field; the KS velocity field such that the largest length scale in the KS field is given by the smallest dimension of the cell. The dissipation cut-off length scale is estimated by the relation $\eta = (\nu^3/\varepsilon)^{1/4} \ [26]$. In contrast to stochastic models that would add a random fluctuation to the unresolved velocity field, here we add a velocity field, which has an underlying structure similar to a turbulent velocity field with finite Reynolds number effect already included by construction \[ 20 \]. The addition of this structure to the unresolved velocity field is equivalent to recovering the SGS that LES has discarded. No other sub-grid model has the ability to model the sub-grid velocity field with an underlying structure as they would usually assume a white noise structure-less velocity field.

We have to be careful about how the KS field is added to the LES field, since there are issues regarding the nature of the KS field near the walls and also when the grid resolution $\Delta$ gets nearer to $\eta$. The strength of the KS field is controlled by the dissipation rate of the resolved velocity, i.e. by the LES velocity field. This allows us to control the contribution of the KS field as the particles approach the wall.

6. RESULTS

In total 10 000 particles were released into the statistically steady LES flow from random locations on a plane ($x-z$) parallel to the walls in the centre of the channel (i.e. $y = L_y/2$) (see, Table II). We then followed their trajectories by integrating the equation of motion (10) for times equivalent to $15L_y/u_0$ and $177L_y/u_0$ depending on the particles relaxation times, so that we obtained a statistically steady distribution of the particle deposition.

The one- and two-particle displacement statistics are shown in Figures 3 and 4, respectively, for LES with (solid line) and without (dotted line) the presence of KS sub-grid model. On the left of these graphs are the results for particles with a lower relaxation time, and on the right are the results for particles with a larger relaxation time. Some differences are observed between
Figure 3. Plot of mean square particle displacements along the \( x \) (top), \( y \) (middle) and \( z \) (bottom) directions, respectively, from a fixed point on the channel mid-plane using LES with KS (solid) and without KS (dotted) sub-grid model. Here, \( \tau_p / t_{t_i} = 0.54 \) (left plots), \( \tau_p / t_{t_i} = 54.54 \) (right plots).

the two scenarios. The differences are due to the presence of a sub-grid flow structure when KS sub-grid model is active. When the sub-grid model is not used the particles only see the LES flow field, which has structures only as small as the resolution of the simulation, i.e. the smallest grid/mesh size. When KS sub-grid model is used the particles see flow structures smaller than the grid resolution. We observed that larger discrepancy between the two models is in the \( y \) and \( z \) directions with the particles with lower relaxation time (Figure 3, left middle and bottom graphs).
Figure 4. Mean square relative particle separation along the $x$ ($\Delta_x = x_1 - x_2$) (top), $y$ ($\Delta_y = y_1 - y_2$) (middle) and $z$ ($\Delta_z = z_1 - z_2$) (bottom) directions, respectively, from a fixed initial separation on the channel mid-plane ($\Delta_y(t = 0) = 0$) using LES with KS (solid) and without KS (dotted) sub-grid model. Here, $\tau_p/\tau_t = 0.54$ (left plots), $\tau_p/\tau_t = 54.54$ (right plots).

It confirms the well-known result that particles with large relaxation time are less sensitive to sub-grid KS structures [23].

In KS, the flow structures have been engineered to behave like a turbulent flow field by construction [19]. Hence, their effects on the particle trajectories are much more realistic. The fact that the difference is greater in the $z$ direction is because the flow is homogeneous in this direction, and
KS can pick up more of the flow physics from the sub-grid, introducing more details than LES. As to the $y$ direction, there is no mean flow in contrast to the $x$ direction, and the flow is less inhomogeneous and more isotropic. Thus, the difference between the two models is also greater in the $y$ than in the $x$ direction. KS does not modify the results so much in the $x$ direction because the flow is strongly dominated by the inhomogeneous feature of the flow, which has already to be picked by LES. Therefore, the effect of the sub-grid fluctuations on the particles in the $x$ direction is not as important as in the $y$ and $z$ directions.

Note that in the $z$ and $y$ directions, there is no mean flow, so eventually for large time, the particle diffusion will follow the well-known random walk (i.e. $\langle y^2 \rangle \sim t$, $\langle z^2 \rangle \sim t$) [47].

The influence of the fine structures present in the sub-grid flow field is more pronounced on the particle relative dispersion, as shown in Figure 4. These statistics are known to be sensitive to the presence of flow structures [41]. Our results are qualitatively similar to what Armenio [17] found using a combination of DNS and LES to study the effects of sub-grid fluctuations on one- and two-particle dispersion in a plane channel turbulent flow.

Figures 3 and 4 also show that the larger the value of $\tau_p$ compared with the local Kolmogorov time scale $\tau_k$, the less sensitive the trajectories are to velocity fluctuations below the sub-grid.

The deposition and distribution of particle statistics are also influenced by the presence of sub-grid flow structures. However, this influence is less obvious for particles with greater relaxation time. Figure 5 shows the particle concentration for particles with greater relaxation time ($\tau_p/\tau_k = 27.27$)

![Particle concentration plots](attachment:image.png)

Figure 5. Particle concentration at $x/h = -0.5$ (top), and 0.6 (bottom) using LES with KS (left plots) and without KS (right). Here $\tau_p/\tau_k = 27.27$. 

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Figure 6. Particle concentration for the finer mesh at $x/h = -0.5$ (top), and 0.6 (bottom) using LES with KS (left plots) and without KS (right). Here $\tau_p/\tau_\eta = 27.27$.

at the left face ($x/h = -0.5$) and near the right face of the rib ($x/h = 0.6$) (cf. Figure 1). In this case, the concentration of particles is similar for both LES and LES + KS. The same results are also shown for a refined mesh, see, Figure 6. With the improved grid resolution, the overall structure of the concentration is still similar for both LES and LES + KS. However, they both show a stronger peak near the smooth wall at $x/h = 0.6$. There are only slight differences between the magnitudes with and without KS, especially near the left face of the rib.

Figure 7 shows particle concentration statistics for particles with a smaller relaxation time ($\tau_p/\tau_\eta = 0.54$). Here, we can see an interesting difference between these two simulations (with and without KS), especially for concentration near the right surface $x/h = 0.6$. Although both simulations show similar concentration pattern, coarse mesh LES gives enhanced deposition compared with the LES with KS model at $x/h = 0.6$ (Figure 7, bottom graphs), shown by a large peak in the particle concentration. However, for a refined mesh, both simulations have picked up the first peak at $x/h = 0.6$, see Figure 8 (bottom graphs) with similar magnitudes. This is because the particles start to feel the smaller eddy structures with the refined mesh, and the two simulations start to converge as the resolution is refined (and approaches DNS). The reason behind the coarse mesh LES flow depositing more particles on the right side of the rib is due to the absence of small-scale eddy structures and the deposition being dominated by the large-scale vortical flow structure present behind the rib [13]. Inclusion of the sub-grid flow structures via the KS model

decreases the amount of deposition, which is similar to the reduction of the deposition of particles near $y/h = 0.6$ via fine mesh LES only flow.

7. DISCUSSION

Our results show that both the deposition and distribution of particle statistics are influenced by the presence of sub-grid flow structures. The smaller the relaxation time of a particle, the more effects the sub-grid model KS has on its trajectories. For particles of greater relaxation time, these effects are negligible. This is in agreement with [17]. The fact that particles with lower relaxation time ($\tau_p / \tau_\eta = 0.54$) are more sensitive to the sub-grid, especially in the directions without mean flow, is significant in terms of our interests in particle deposition in airways. These directions correspond to the walls where particle deposition occurs. And it is generally believed that inhaled micron-sized particles with low relaxation time (diameter 2–5 $\mu$m) deposit primarily by inertial impaction and sedimentation, especially in the relatively large tracheo-bronchial airways [48]. Therefore, we believe that the sub-grid effects should indeed be considered when modelling particle deposition in the turbulent airway flows.

We have successfully adapted KS as a sub-grid model for a LES simulation of flow over ribbed wall channel. This combined approach is used for particle tracking in a turbulent flow. The current
Figure 8. As in Figure 7, but with the finer mesh for $\tau_p/t_h = 0.54$.

Our work differs from the existing literature in that this approach can overcome the difficulties that LES alone has in resolving the sub-grid eddies around or below the filter cut-off [14–16]. It can also be used for inhomogeneous flows and flows with boundary conditions, which KS alone cannot do. One open question to be addressed in the KS modelling is when to switch the KS off near the wall. In this paper, the KS model is controlled by the cut-off energy dissipation from LES, which becomes small near the wall. The zonal LES model we used switches to a RANS model near the wall, thus the KS is also switched off at the same time. This may be responsible for the unexpected peak near the top wall ($y/h \sim 10$) on the right of the rib (Figure 6, bottom graphs), which was picked up both by LES+KS and LES with a finer mesh. This is because the number of cells over which RANS is used increases for the finer mesh, and the effect of RANS is enhanced near the wall. This weakness could be overcome by more advanced KS models, which can deal with boundary conditions, see for example [49]. Clearly, more detailed studies on the general choice of KS switch/modelling near the wall are desired. We have chosen to use a validated case (ribbed channel flow) because the focus here is on adapting KS to LES. Needless to say, for general complex problems, a reliable LES model is the pre-requisite for the combined LES+KS approach.

Our work is a first step towards understanding the effects of sub-grid modelling on Lagrangian particle dynamics. In this context, KS provides a conveniently malleable tool. This enables one to numerically model the small-scale turbulent flow structure at will. With this method, we can explore how various properties of this flow structure relate to or determine the turbulent particle statistics. In future, LES with KS type of sub-grid modelling may be applied to more complicated...
flow domain, such as the particle deposition in the human airway in order to understand more
detailed effects of turbulent flow structure.

8. CONCLUSIONS

The effects of LES sub-grid flow structure on particle motion have been investigated using a novel
sub-grid model KS. This is the first time this type of combined modelling has been carried out
in the context of LES of a turbulent flow field with boundaries. The KS model introduces flow
structures with finite range of scales suitable for a finite Reynolds number turbulence, which is in
contrast to stochastic models applicable only to an infinite Reynolds number turbulent flow, where
it is necessary to tune a number of coefficients to match the large-scale flow domain. In KS, we
have no free parameters except the power law of the energy spectrum. All the other parameters
of the model are fixed by the resolved LES flow field. We have shown the influence of SGS on
particle motion through the differences seen in the particle dispersion and deposition statistics.
This influence is more important for particles with smaller relaxation time.

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EFFECTS OF LES SUB-GRID FLOW STRUCTURE